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Non-perturbative QCD by lattice simulations

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Summary. — We present a brief overview of the status of lattice QCD computations for the study of strong interactions in the non-perturbative regime. We focus in particular on the computational requirements and on results concerning the phase diagram of QCD at finite temperature and baryon density.

PACS 11.15.Ha – Lattice gauge theory.
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1. – Introduction

Nowadays, Quantum ChromoDynamics is accepted as the quantum field theory which describes strong interactions. Asymptotic freedom guarantees the applicability of a perturbative expansion at energies much larger than $\Lambda_{\rm QCD} \sim 200\,\text{MeV}$. At low energies, instead, the theory is non-perturbative: the only known computational scheme of the theory in this regime was proposed by K. G. Wilson more than 30 years ago [1] and is based on a Monte Carlo stochastic computation of the path integral of the theory, regularized in a gauge invariant on an Euclidean space-time lattice.

Let us consider the partition function of QCD at finite temperature T on a finite spatial volume V. That can be given a regularized path integral representation as follows:

$$Z(V,T) = \int \mathcal{D}U\mathcal{D}\psi\mathcal{D}\bar{\psi} e^{-(S_G[U]+\bar{\psi}M[U]\psi)} = \int \mathcal{D}U e^{-S_G[U]} \det M[U]. \tag{1}$$

Here $U_\mu(n) \simeq \mathcal{P}\exp(i\int_n^{n+\mu} A_\mu \mathrm{d}x_\mu)$ are the elementary non-Abelian parallel transports from lattice site n to the nearest neighbor site $n+\mu$ (we assume a hypercubic lattice), which belong to the $SU(3)$ gauge group (gauge link variables); S_G is a regularization of the pure gauge part of the QCD action, $(1/4)\int \mathrm{d}^4x F^a_{\mu\nu}F^{\mu\nu}_a$, $\psi(n)$ are the fermionic variables and $\bar{\psi}M[U]\psi$ is a regularization of $\sum_f \int \mathrm{d}^4x \bar{\psi}_f\,(D^\mu\gamma_\mu + m_f)\psi_f$.

The final expression, which is obtained after integration over the fermionic Grassmann variables, is computable by numerical Monte Carlo simulations if $e^{-S_G[U]}\det M[U]$ is

a real and positive quantity, which can be interpreted as a probability distribution over the gauge configurations U.

In the above expressions, the time extension, $N_t a$ (a being the lattice spacing), is taken equal to the inverse of the physical temperature T, with periodic (antiperiodic) boundary conditions (b.c.) for bosonic (fermionic) variables. The spatial extension, $L_s a$, is taken much larger than $1/T$, to approximate the thermodynamical limit, and one is free to choose the preferred b.c. in this case. The lattice spacing a does not enter the lattice formulation explicitly, but is tunable through the bare gauge coupling g_0: asymptotic freedom guarantees that the continuum limit is reached as $g_0 \to 0$.

Lattice simulations can provide essential insight into the QCD phase diagram (as discussed in more detail in sect. **2**) and, in the limit $N_t a \to \infty$, into zero T physics, including the non-perturbative structure of the QCD vacuum state. Useful information comes, for instance, from the asymptotic behaviour of (Euclidean) time correlators of suitable field operators:

$$\lim_{\tau\to\infty} \langle 0|\mathcal{O}(\tau)\mathcal{O}(0)|0\rangle = \lim_{\tau\to\infty} \sum_n |\langle n|\mathcal{O}(0)|0\rangle|^2 e^{-\tau(E_n - E_0)} \sim |\langle n_{\mathcal{O}}|\mathcal{O}(0)|0\rangle|^2 e^{-\tau(E_{n_{\mathcal{O}}} - E_0)}$$

where $|n_{\mathcal{O}}\rangle$ is the lowest energy state coupled to the vacuum through $\mathcal{O}$. In this way, depending on the choice of $\mathcal{O}$, one can obtain information about hadron masses or interaction potentials, by measuring $E_{n_{\mathcal{O}}} - E_0$, or about matrix elements $|\langle n_{\mathcal{O}}|\mathcal{O}(0)|0\rangle|^2$ which may be interesting for Standard Model phenomenology.

Of course lattice predictions come with systematic uncertainties, related to the finite lattice spacing and lattice size (UV and IR cutoff), which however can be monitored and kept under control. In principle one would like to have a lattice spacing much shorter than the shortest physical scale into play, and a lattice size aL_s much larger than the inverse pion mass. That would require L_s to be at least of $O(10^2)$, corresponding to a system of about 10^9–10^{10} stochastic variables.

The required computational effort was completely out of the reach of early lattice computations, which could rely on a computational power well below 1 Gflop, *i.e.* 10^9 flops (floating point operations per second). Therefore early computations were constrained to small and coarse lattices and typically neglected the contribution of the fermion determinant in eq. (1) (quenched approximation), that represents the most expensive task in lattice simulations. Nowadays we are entering the era of Petaflop (10^{15} flops) supercomputers and reliable and precise computations are at hand (see *e.g.* ref. [2] for a recent determination of the light hadron masses at a few percent level of accuracy).

However we still need some help from chiral perturbation theory to extrapolate to physical values of the dynamical quark masses, since pion masses used in present lattice computations are hardly below 200 MeV. Analogous problems are encountered when studying heavy meson physics, *e.g.* B-physics (see *e.g.* ref. [3] for a recent discussion): feasible valence quark masses are limited by the UV cutoff, which is not larger than a few GeV, and one has tipically to rely on extrapolations based on heavy quark effective theories.

The increase in computational power is not the only way to make progress in lattice QCD simulations: algorithmic and discretization improvements play a fundamental role. Consider for instance the computational difficulty for obtaining 100 statistically independent gauge configurations in the case of 2 dynamical quark flavors in the Wilson

discretization. In 2001 that was estimated as [4]

$$3.10 \left(\frac{aL_s}{3\,\mathrm{fm}}\right)^5 \left(\frac{L_s}{2N_t}\right) \left(\frac{0.2}{\hat{m}/m_s}\right)^3 \left(\frac{0.1\,\mathrm{fm}}{a}\right)^7 \mathrm{TFlop}\cdot\mathrm{year} \tag{2}$$

where $\hat{m}/m_s$ is the ratio of the light to strange quark mass. The same estimate has dropped to

$$0.03 \left(\frac{aL_s}{3\,\mathrm{fm}}\right)^5 \left(\frac{L_s}{2N_t}\right) \left(\frac{0.2}{\hat{m}/m_s}\right) \left(\frac{0.1\,\mathrm{fm}}{a}\right)^6 \mathrm{TFlop}\cdot\mathrm{year} \tag{3}$$

after algorithmic and technical improvements, as reported in ref. [5]. Even using eq. (3), a quick computation shows that, in order to obtain a large sample (say 10^3 configurations), with physical parameters and an UV cutoff $a^{-1} > 5\,\mathrm{GeV}$, in a reasonable time, one needs computer resources at least at the Petaflop scale.

2. – Results on the QCD phase diagram

The main aim of numerical studies of finite temperature QCD is to map the different possible phases of strongly interacting matter and their physical properties: the location and the nature of the phase transitions from a low-T confined regime with spontaneous breaking of chiral symmetry to a deconfined and chirally symmetric high-T phase, are of obvious interest for heavy-ion experiments dedicated to the study of the quark-gluon plasma and for understanding the evolution of the Universe in its early stages.

The numerical task, as compared with zero T simulations, is simplified, on the one hand, because of the compactified temporal direction which makes the system smaller, but it is harder, on the other hand, since several different simulations are needed at different values of T around the transition and on different spatial volumes, in order to follow the approach to the thermodynamical limit and determine the universal critical behaviour of the system (finite size scaling).

Numerical simulations of quenched QCD have shown that the pure $SU(3)$ gauge theory undergoes a first-order deconfining transition [6] associated with the spontaneous breaking of the center symmetry. When dynamical quarks are taken into accout, the scenario is less simple. Exact symmetries of QCD are known only in the limit of zero (chiral symmetry) or infinite (center symmetry) quark masses: in the generic case no other symmetry is presently known, which may change its realization at the transition, hence there is no need for a real phase transition and one may have a rapid analytic change of physical properties instead. On the other hand, knowing from numerical simulations if deconfinement is associated to a real transition can teach us if it is sensible to search for some other, yet unknown symmetry of QCD.

In principle the nature of the transition can depend on the values of the quark masses, so that it is necessary to study also the flavor spectrum dependence. In fig. 1 (left) we report the commonly accepted scenario for the order of the transition as a function of the up and down quark masses, which are assumed to be degenerate, and of the strange quark mass. The phase transition is of first order in restricted regions of very high or very low quark masses, which are limited by second order boundaries. Present numerical data are consistent with a crossover in the case of physical quark mass [7]. There are still unsettled issues: in the limit of two massless flavors (upper-left corner) chiral symmetry

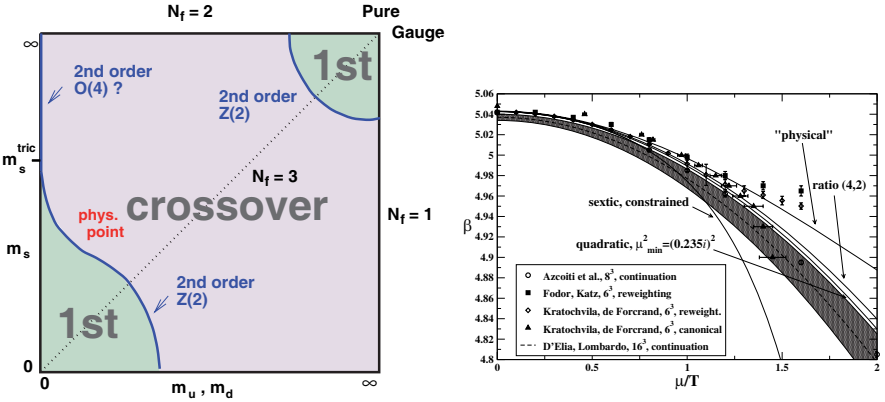

Fig. 1. – Nature of the QCD transition as a function of the quark-mass spectrum (left) and dependence of the pseudocritical coupling β_c on the chemical potential as obtained by different techniques and extrapolations in $N_f = 4$ QCD (right).

implies the existence of a chiral phase transition, which should be in the $O(4)$ universality class if it is of second order [8] but can be of first order otherwise: present numerical results have not confirmed the $O(4)$ universality class, but they have not yet provided conclusive evidence for a first order transition [9].

The numerical study of the QCD phase diagram becomes much more difficult when a finite baryon density is taken into account: this is necessary to correctly describe the physics of heavy ion collisions and of certain astrophysical objects. The interesting information concerns how the critical temperature T_c and the nature of the transition change as a function of the baryon chemical potential μ_B. In particular, if a crossover is present at $\mu_B = 0$, it is possible that, increasing μ_B, it may turn into a first order, going through a second order critical endpoint which may have significant experimental signatures [10]. An even richer phase structure is expected in the region of small temperatures and high densities (see ref. [11] for a recent review).

Unfortunately, numerical simulations are not feasible in presence of a finite baryon chemical potential, since the fermion determinant appearing in eq. (1) becomes complex and does not permit a probabilistic interpretation of the functional integral measure (sign problem). Reliable numerical results can be obtained only in a restricted region of high temperatures and small chemical potentials, where approximate solutions to the problem can be found, among which reweighting techniques [12, 13], analytic continuation from imaginary chemical potentials [14-16] and Taylor expansion techniques [17, 18].

In fig. 1 (right) we show a comparison (see ref. [19]) of the critical line $T_c(\mu_B)$ determined in the case of four degenerate flavors by different techniques (the pseudocritical coupling β_c is reported in place of T_c, which is a monotonically increasing function of T_c): consistency among different determinations is obtained only as long as $\mu/T \leq 1$ ($\mu \equiv \mu_B/3$). The same techniques have failed, up to now, to provide clear and consistent evidence for the presence and location of a critical endpoint in the case of $N_f = 2 + 1$ QCD.

Contrary to the case of a finite baryon density, no technical difficulties are encountered in the numerical study of the QCD phase diagram in presence of other external

parameters which may be relevant to phenomenology, like for instance an (electro-) magnetic background field [20].

3. – Perspectives

Nowadays, apart from some hard problems, like the numerical study of QCD at finite baryon density, we are entering the era in which Monte Carlo lattice simulations can really provide a tool to systematically compute QCD.

In this scenario, an essential requirement is the availability of adequate computational resources. The Petaflop scale will represent a benchmark, in the next few years, for most groups willing to play a significant role in the field. The italian lattice community has always played a major role and has a renowned experience in the design of dedicated supercomputing machines (APE, APE100, APEmille and apeNEXT projects): present available resources, mostly represented by apeNEXT facilities, are at the scale of 10 Teraflops and largely undersized for future research plans and with respect to the resources available to other lattice groups in the world. This gap will hopefully be filled in the next couple of years by ongoing projects for future dedicated machines (AuroraScience and apeNET+).

In contexts where large scale funding for supercomputing are not available, possible alternatives can be found in Graphics Processor Units (GPUs), which represent an optimal cost effective solution [21-23], with a single GPU providing computer power at the Teraflop scale. They are surely an optimal choice for mid-term solutions to computational requirements and may be at the basis of possible future large scale supercomputers: the recently appeared second fastest supercomputer in the world (*Nebulae*, National Supercomputing Centre, Shenzhen, China) is already partially based on GPU accelerators.

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